The experimentally determined values of spectral specular reflectance of various materials and their correlation with computed values have been extensively reported in the literature [2–4]. But in the case of computation of spectral diffuse reflectance there exists 3 different approaches [5–7], which led to 6 different models. So, every time, selecting a particular model for a particular material and performing calculation by usual way is very cumbersome and also time consuming. Thus, as an easy alternative, a computer code is developed in *C* language for the evaluation of both diffuse as well as specular reflectance of any material for all the wavelengths.

Spectral specular reflectance follows Snell's law of reflection and can be determined from Fresnel's relation [2]. Regarding diffuse reflectance (R_{diff}) in general, the conventional Kubelka-Munk (K-M) theory is obeyed and is given by the following relation :

$$(1 - R_{diff})^2/(2R_{diff}) = (K/S). \quad (3)$$

or

$$R_{diff} = [1 + (K/S)] - [(1 + K/S)^2 - 1]^{1/2}, \quad (4)$$

where, K and S are the absorption and scattering coefficients respectively of the material.

The advanced statistical theory defines diffused reflectance as

$$R_{diff} = \{(1 + r^2 - t^2) + [(1 + r^2 - t^2)^2 - 4r^2]^{1/2}\}/2r, \quad (5)$$

where, t and r are respectively the transmittance and reflectance of a single particle and can be determined through modified particle model theory (MPMT), plane parallel plate model (PPPM) and Melamed theory (MT). $T(\lambda)$, $R(\lambda)$, t, r, K and S are all wavelength dependent. As stated above, out of 3 different approaches leading to 6 different models, only three models for two approaches *i.e.* statistical and differential equation (K-M theory) approach have been dealt in this work because of their practical importance. Though, the details are discussed by Simmons [6,7], here, only the expressions showing the r and t dependence on other parameters for all models referred above and other expressions used in the computer coding are given and defined.

For Modified Particle Model Theory (MPMT), the expression is :

$$r = (3m_e/4) + (T/2)[(1 - m_e)(1 - m_i)][(1 - m_iT)^{-1} - \{(1 - m_i/2)(1 - m_e/2)(1 + m_iT/2)^{-1}\}, \quad (6)$$

$$t = (m_e/4) + (T/2)[(1 - m_e)(1 - m_i)][(1 - m_iT)^{-1} + \{(1 - m_i/2)(1 - m_e/2)(1 + m_iT/2)^{-1}\}. \quad (7)$$

For Plane Parallel Plate Model (PPPM), the expression is :

$$r = r_o + [\{(1 - r_o)^2 r_o \exp(-\alpha d)\}\{1 - r_o^2 \exp(-2\alpha d)\}^{-1}], \quad (8)$$

$$t = \{(1 - r_o)^2 \exp(-\alpha d)\}\{1 - r_o^2 \exp(-\alpha d)\}^{-1}. \quad (9)$$

For Melamed Theory (MT), the expression is :

$$r = m_e + [\{(1 - m_e)(1 - m_i)M/2\}\{1 - m_iM\}^{-1}]. \quad (10)$$

$$t = \{(1 - m_e)(1 - m_i)M/2\}\{1 - m_iM\}^{-1}, \quad (11)$$

where various terms used in these expressions are defined as :

$$m_e = (1/2)[\{n^2 \cos\theta - (n^2 - \sin^2\theta)^{1/2}\}\{n^2\cos\theta + (n^2 - \sin^2\theta)^{1/2}\}^{-1}]^2 + (1/2)[\{\cos\theta - (n^2 - \sin^2\theta)^{1/2}\}\{\cos\theta + (n^2 - \sin^2\theta)^{1/2}\}^{-1}]^2, \quad (12)$$

$$m_i = 1 - \{(1 - m_e)n^{-2}\}. \quad (13)$$

$$r_o = \{(1 - n)(1 + n)^{-1}\}^2. \quad (14)$$

$$M = 2\{1 - (\alpha d + 1)\exp(-\alpha d)\}\{(\alpha d)^{-2}\}, \quad (15)$$

$$R_s = [(\cos\theta - u)^2 + v^2][(\cos\theta + u)^2 + v^2]^{-1}. \quad (16)$$

$$R_p = [\{(n^2 - k^2)\cos\theta - u\}^2 + \{2nk\cos\theta - v^2\}][\{(n^2 - k^2)\cos\theta + u\}^2 + \{2nk\cos\theta + v^2\}]^{-1}, \quad (17)$$

$$u^2 = [\{n^2 - k^2 - \sin^2\theta\} + \{(n^2 - k^2 - \sin^2\theta)^2 + 4n^2k^2\}^{1/2}]/2, \quad (18)$$

$$v^2 = [\{n^2 - k^2 + \sin^2\theta\} + \{(n^2 - k^2 + \sin^2\theta)^2 + 4n^2k^2\}^{1/2}]/2. \quad (19)$$

The developed computer code (Flow Chart shown in Appendix) efficiently handles all the above said relations.

In order to assess the validity of the software for R_{spec}, the values computed by using the computer code were compared with those of experimental values obtained on both surfaces polished germanium (Figure 1). Since absorptance, $A \approx 0$ for this case, their spectral transmittance values can also be determined from their R_{spec} values by using eq. (2). Experimental work on various materials for the determination of their diffuse reflectance is in progress. In order to verify the reliability of software for R_{diff}, the results obtained through this code was compared with those calculated by conventional means for unpolished germanium (Figure 2).

The features of this code are

(i) The input data such as wavelength, refractive index (n) and extinction coefficient (k) are stored in separate files.

(ii) Even though, the specular reflectance values calculated for the incident angle $\theta \approx 10°$ are shown in Figure 1, specular reflectance values as per requirement can be calculated for any incident angle.

(iii) The diffuse reflectance values, as per the model selected, are stored in corresponding files. Since grain size plays an important role in determining R_{diff}, the calculation done for various grain size values can be updated at any time. Therefore, much of the calculation time as well as redundancy are eliminated.

(iv) Results for the diffuse reflectance calculation performed for different models are stored in separate files. Due to the efficient file management, results thus stored are highly independent, which provides security even if changes are necessary.

A computer code is developed for the simultaneous calculation of spectral specular as well as spectral diffuse reflectance, which provides good accuracy and reliability. Though, the agreement between the experimental and calculated R_{spec} values (Figure 1) is within the measurement accuracy of the spectrophotometer, a systematic lower experimental value beyond 4 μm may be because of reflection losses within the sample. Also, a wide disagreement at 16μm is because of selective absorption due to Ge–Ge

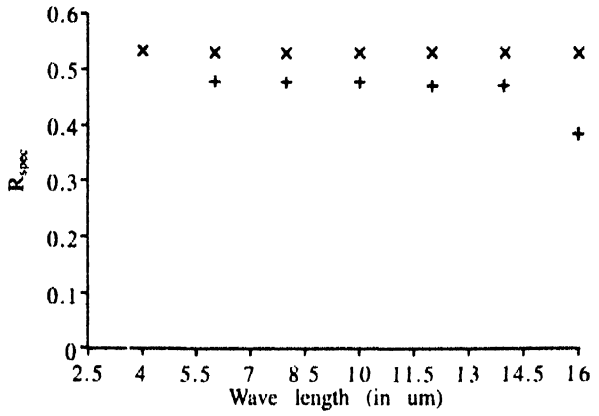

Figure 1. Specular reflectance values of both surfaces polished germanium; (a) calculated (× × ×) and (b) experimental (+ + +), at an angle of incidence = 10°.

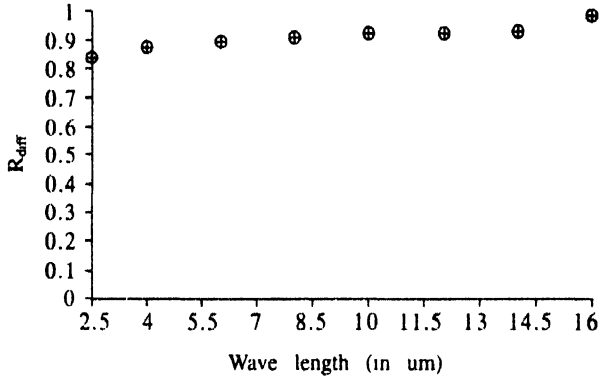

Figure 2. Diffuse reflectance value of germanium by Modified Particle Model Theory (MPMT) for grain size $d = 60\mu$m : Computed using (a) Microsoft-Excel (o o o); and (b) the program discussed here (+ + +).

lattice vibration and/or Ge–oxygen impurity, which has not been taken in to account for calculated values. The diffuse reflectance value computed by using this code is also in good agreement with those computed by using other means (Figure 2). Because of the independent storage of data, results are efficiently protected.

References

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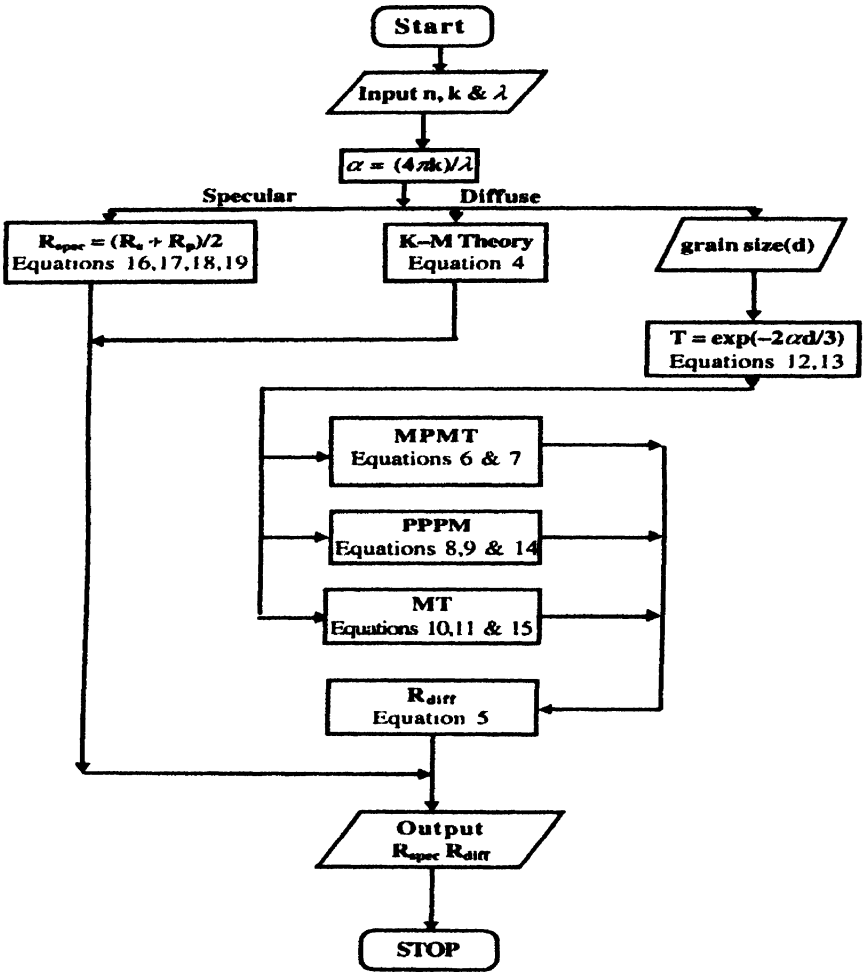
APPENDIX


Start
Input n, k & λ
α = (4πk)/λ
Specular
Diffuse
R_spec = (R_s + R_p)/2
Equations 16,17,18,19
K–M Theory
Equation 4
grain size(d)
T = exp(–2αd/3)
Equations 12,13
MPMT
Equations 6 & 7
PPPM
Equations 8,9 & 14
MT
Equations 10,11 & 15
R_diff
Equation 5
Output
R_spec R_diff
STOP